

## **ADAPTIVE MODELING FOR MULTI-SCALE METHODS**

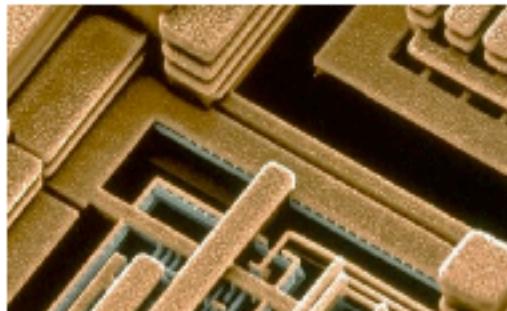
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The University of Texas at Austin

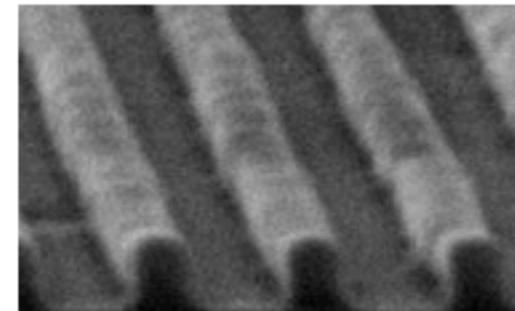
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**AtC Coupling Methods Workshop  
Sandia National Laboratories**

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**Albuquerque, NM  
March 20-21, 2006  
Supported by DOE**



## OUTLINE

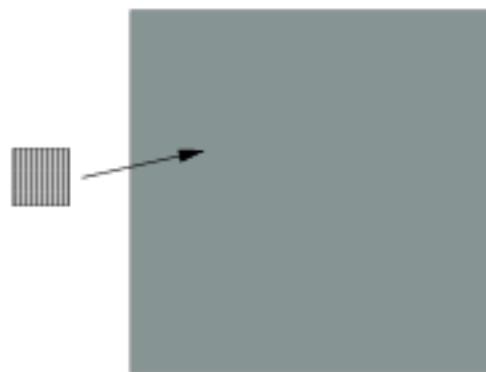
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- 1. Model Adaptivity for Multi-scale Problems: Motivation**
- 2. Goal-Oriented Error Estimation and Control**
- 3. Examples:**
  - **Quasi-Continuum Method**
  - **Molecular Dynamics**
- 4. Step-and-Flash Imprint Lithography**
- 5. Concluding Remarks**

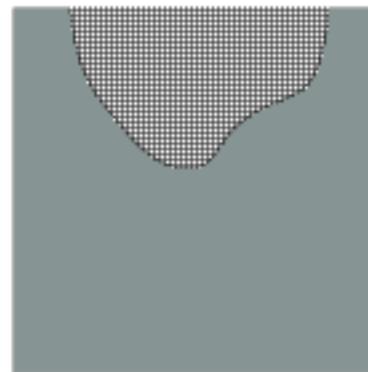
## 1. MULTI-SCALE MODELING AND ADAPTIVITY

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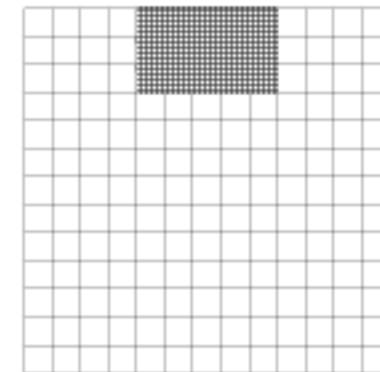
1. **Hierarchical** – S. Hao, et al, CMAME, 2004.
2. **Concurrent** – MAAD/CLS, CADD, BSM, PMM, BDM, Goals
3. **Hybrid** – QC, HMM, Goals



Hierarchical



Concurrent



Hybrid

**Remark:** More precise classifications may be needed

## 2. GENERAL FRAMEWORK FOR ADAPTIVE MODELING

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A physical event  
is depicted by a  
mathematical model:

$$A(u) = F, \quad \text{in } V'$$

A goal is to calculate a  
quantity of interest:

$$Q(u) = ?$$

$$Q: V \longrightarrow \mathbb{R}$$

The problem is generally  
unsolvable, so it is replaced  
by a surrogate problem:

$$A_0(u_0) = F_0, \quad \text{in } V'$$

1) The (wrong) value of  $Q$  is:

$$Q(u_0) \neq Q(u)$$

2) Can we estimate the error?

$$\mathcal{E} = Q(u) - Q(u_0)$$

3) Can we adapt the surrogate  
model and control the error?

## 2. A REVIEW OF GOAL-ORIENTED ERROR ESTIMATION

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**Weak form of model problem:**

Let  $B(u; v) = \langle A(u), v \rangle$  and  $F(v) = \langle F, v \rangle$ . Then

Find  $u \in V$  such that  $B(u; v) = F(v), \quad \forall v \in V$

**Optimal Control Problem for Quantity of Interest  $Q$ :**

$$Q(u) = \inf_{v \in M} Q(v)$$

$$M = \{v : B(v; w) = F(w), \forall w \in V\}$$

Then

$$B(u; q) = F(q), \quad \forall q \in V \text{ (Primal)}$$

$$B'(u; v, p) = Q'(u; v), \quad \forall v \in V \text{ (Dual)}$$

## 2. ERROR FUNCTIONS AND RESIDUALS

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**Recall:**

$$Q'(u; v) = \lim_{\theta \rightarrow 0} \theta^{-1} [Q(u + \theta v) - Q(u)]$$

$$B'(u; v, w) = \lim_{\theta \rightarrow 0} \theta^{-1} [B(u + \theta v; w) - B(u; w)]$$

**Let  $(u_0, p_0)$  be an arbitrary pair on  $V \times V$ .**

**Denote the errors:**

$$e_0 = u - u_0, \quad \varepsilon_0 = p - p_0$$

**and the residuals:**

$$\mathcal{R}(u_0; q) = F(q) - B(u_0; q), \quad q \in V$$

$$\overline{\mathcal{R}}(u_0, p_0; v) = Q'(u_0; v) - B'(u_0; v, p_0), \quad v \in V$$

## 2. ERROR IN THE QUANTITY OF INTEREST

**THEOREM<sup>1</sup>:**

**Given the solution pair  $(u, p)$ , then for any  $(u_0, p_0)$ ,**

$$Q(u) - Q(u_0) = \mathcal{R}(u_0; p) + \Delta(e_0, \varepsilon_0)$$

**where**

$$\begin{aligned} \Delta(e_0, \varepsilon_0) &= \frac{1}{2} \int_0^1 \left[ Q'''(u_0 + se_0; e_0, e_0, e_0) \right. \\ &\quad - B'''(u_0 + se_0; e_0, e_0, e_0, p_0 + s\varepsilon_0) \\ &\quad \left. - 3B''(u_0 + se_0; e_0, e_0, \varepsilon_0) \right] (s-1)s \, ds \\ &+ \int_0^1 \left[ B''(u_0 + se_0; e_0, e_0, p_0 + s\varepsilon_0) \right. \\ &\quad \left. - Q''(u_0 + se_0; e_0, e_0) \right] \, ds \end{aligned}$$

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<sup>1</sup>Oden & Prudhomme, *J. Comp. Phys.* (2002).

<sup>2</sup>For FEM's, see Oden & Prudhomme (1999), Rannacher & Becker (2001).

## 2. THE SURROGATE MODEL

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Coarse or Surrogate Primal and Dual problems:

$$\begin{aligned} B_0(u_0; q) &= F_0(q), & \forall q \in V_0 \\ B'_0(u_0; v, p_0) &= Q'_0(u_0; v), & \forall v \in V_0 \end{aligned}$$

where  $V_0 \subseteq V$  (analysis of modeling error).

Discrete Primal and Dual problems:

$$\begin{aligned} B_0(u_0^h; q^h) &= F_0(q^h), & \forall q^h \in V_0^h \\ B'_0(u_0^h; v^h, p_0^h) &= Q'_0(u_0^h; v^h), & \forall v^h \in V_0^h \end{aligned}$$

where  $V_0^h \subset V_0$  (analysis of discretization error).

## 2. ERROR ESTIMATION

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$$Q(u) - Q(u_0) \approx \mathcal{R}(u_0; p) \approx \mathcal{R}(u_0; \tilde{p})$$

Note that  $u_0$  is rarely computed exactly. In general, only an approximation  $u_0^h$  to  $u_0$  is available. In this case, we have:

$$Q(u) - Q(u_0^h) \approx \mathcal{R}(u_0^h; \tilde{p})$$

$$Q(u_0) - Q(u_0^h) \approx \mathcal{R}_0(u_0^h; \tilde{p}_0)$$

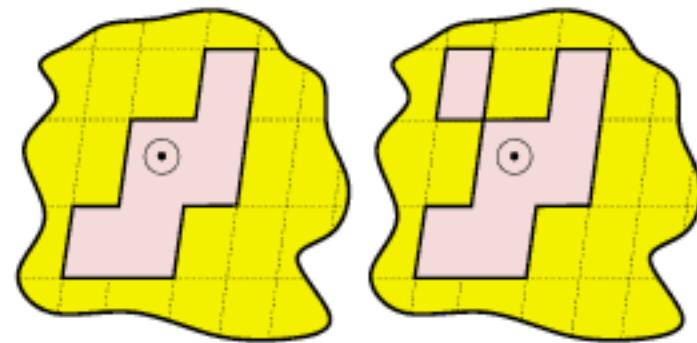
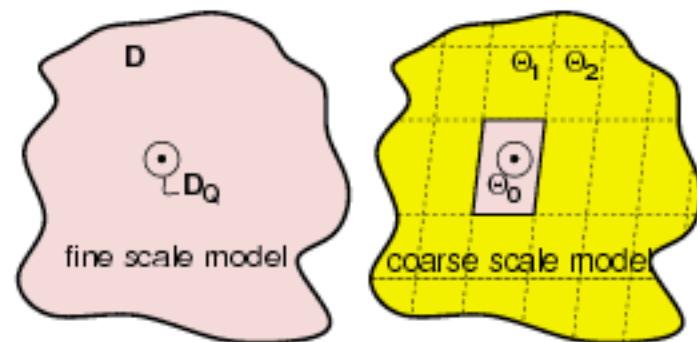
and

$$\underbrace{Q(u) - Q(u_0)}_{\text{modeling error}} = \underbrace{(Q(u) - Q(u_0^h))}_{\text{total error}} - \underbrace{(Q(u_0) - Q(u_0^h))}_{\text{discretization error}}$$

## 2. THE GOALS ALGORITHMS (2 SCALE SYSTEM)

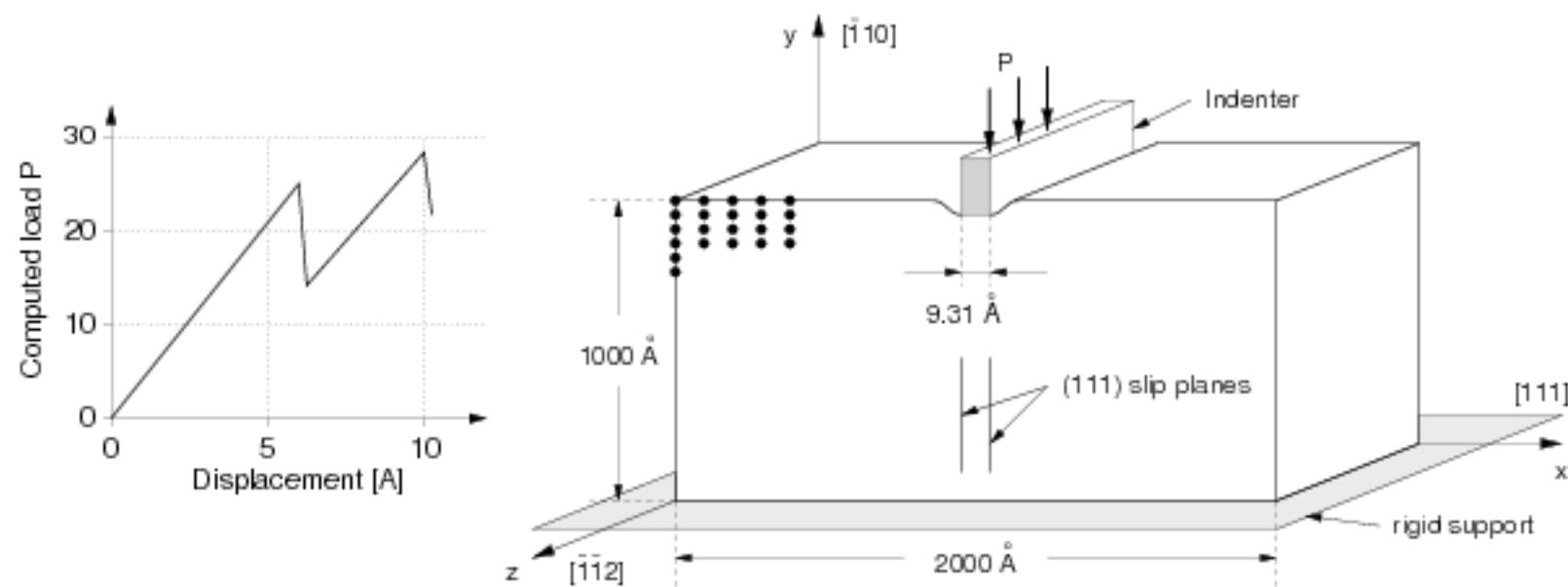
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1. Let  $D \subset \mathbb{R}^d$  and let  $\{\Theta\}_{j=0}^k$  be a partition of  $D$ .
2. Compute  $u_0$  and  $\mathcal{R}(u_0, p_0) \approx \mathcal{E}(u_0)$ .
3. Check  $|\mathcal{E}(u_0)| \leq \delta_{\text{TOL}}$ .
4. Compute corrections  $(\tilde{u}, \tilde{p})$  of  $(u_0, p_0)$  and continue until  $|\mathcal{E}(u_0)| \leq \delta_{\text{TOL}}$ .



### 3. MOLECULAR STATIC EXAMPLE\*

**Nano-indentation of a thin aluminium film to study the initial stages of plastic deformation under the action of an indenter.**



\*Tadmor, Miller, Phillips, and Ortiz, J. Mat. Res. 14, (1999)

\*Phillips, Rodney, Shenoy, Tadmor, and Ortiz, Model. Simul. Mat. Sci. Eng. 7 (1999)

### 3. THE BASE MODEL

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**Goal of molecular statics:**

**Find  $u \in \mathcal{V} \subset (\mathbb{R}^d)^N$  that minimizes the total potential energy, that is**

$$E_p(u) = \min_{v \in \mathcal{V}} [E_p(v)] = \min_{v \in \mathcal{V}} \left[ - \sum_{i=1}^N f_i \cdot v_i + \sum_{k=1}^N E_k(v) \right]$$

**where:**

- $f_i$  = external applied load on atom  $i$
- $E_k$  = energy of atom  $k$  from interatomic potentials by the Embedded Atom Method (EAM)\*

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\*Daw & Baskes (83), Ercolessi & Adams (94).

### 3. THE BASE MODEL

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Find  $u \in \mathcal{V}$  and  $p \in \mathcal{V}$  such that

$$\text{(Primal problem)} \quad \mathcal{B}(u; v) = \mathcal{F}(v), \quad \forall v \in \mathcal{V}$$

$$\text{(Dual problem)} \quad \mathcal{B}'(u; v, p) = Q'(u; v), \quad \forall v \in \mathcal{V}$$

where

$$\mathcal{B}(u; v) = \sum_{i=1}^N \left[ \sum_{k=1}^N \frac{\partial E_k}{\partial u_i}(u) \right] \cdot v_i$$

$$\mathcal{F}(v) = \sum_{i=1}^N f_i \cdot v_i$$

and

$$\mathcal{B}'(u; v, p) = \sum_{j=1}^N \sum_{i=1}^N v_j \cdot \left[ \sum_{k=1}^N \frac{\partial^2 E_k}{\partial u_j \partial u_i}(u) \right] \cdot p_i$$

### 3. ERROR ESTIMATION

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Define an intermediate triangulation such that  $R < \tilde{N} \ll N$  and the extension operator  $\tilde{\Pi} : W \rightarrow \tilde{V}$ .

**Surrogate dual problem:**

Find  $\tilde{p} \in \tilde{V}$  such that

$$\tilde{\mathcal{B}}'(\tilde{\Pi}u_0; \tilde{v}, \tilde{p}) = \tilde{Q}'(\tilde{\Pi}u_0; \tilde{v}), \quad \forall \tilde{v} \in \tilde{V}$$

**Error estimator:**

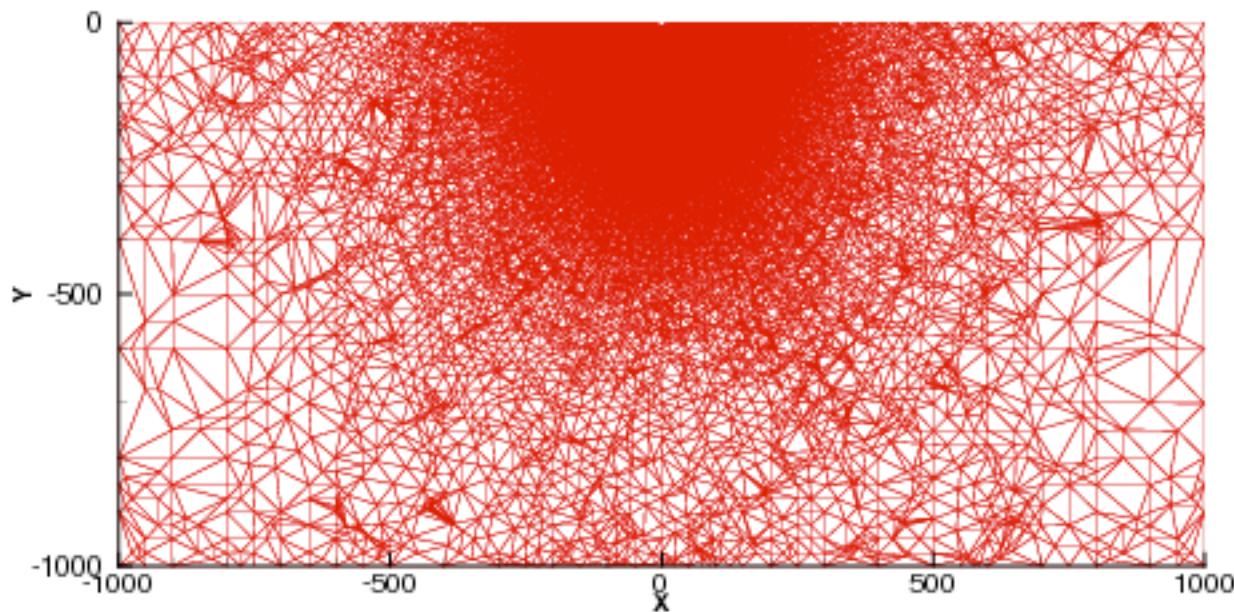
$$\eta = \tilde{R}(\tilde{\Pi}u_0; \tilde{p}) = \sum_{i=1}^{\tilde{N}} \tilde{r}_i(\tilde{\Pi}u_0) \cdot \tilde{p}_i \approx Q(u) - Q_0(u_0)$$

The quantity  $\eta$  can be decomposed into elementwise contributions  $\eta_K$  such that:

$$\eta = \sum_{K=1}^{N_e} \eta_K = \left| \frac{1}{|K|} \int_K \sum_{i=1}^3 \eta_i^K \phi_i(x) \, dx \right|$$

### 3. BASE MODEL SOLUTION

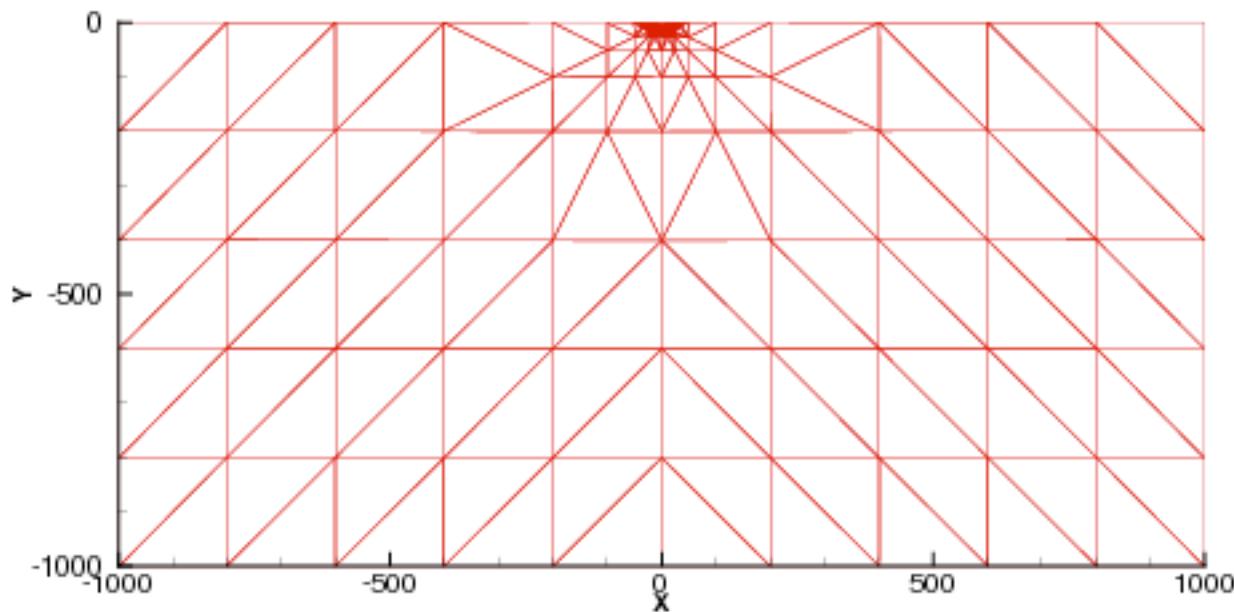
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**Finite element triangulation for the base model solution  
at load step 26:  
the mesh has 40554 active atoms.**

### 3. QUASICONTINUUM SOLUTION

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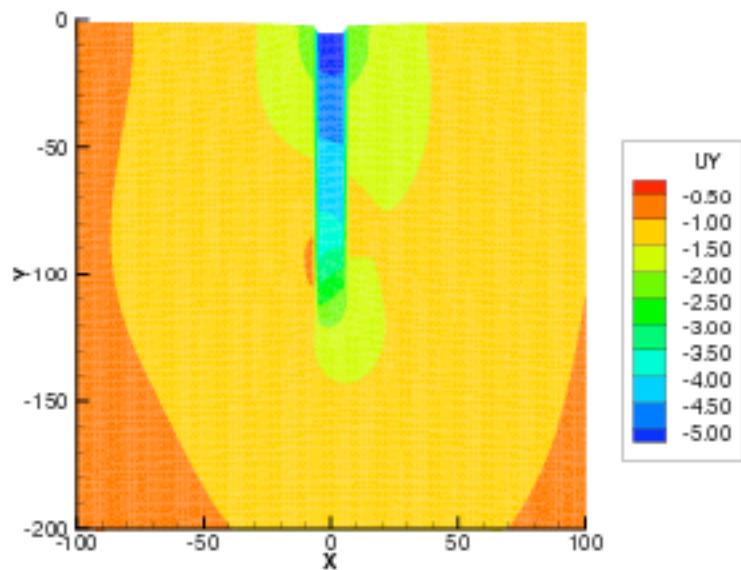


**Finite element triangulation for the QC solution  
at load step 25:  
the mesh has 492 active atoms.**

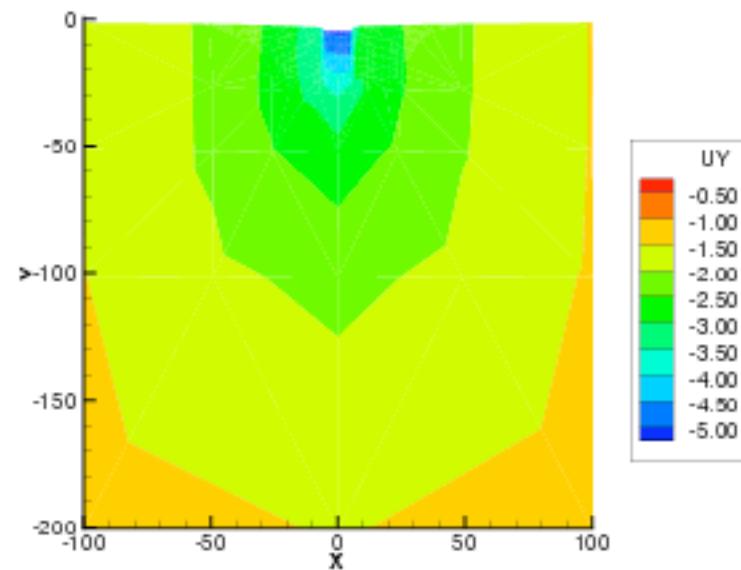
### 3. BASE AND QC SOLUTIONS

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Displacement in  $y$ -direction  
at dislocation nucleation



Base solution

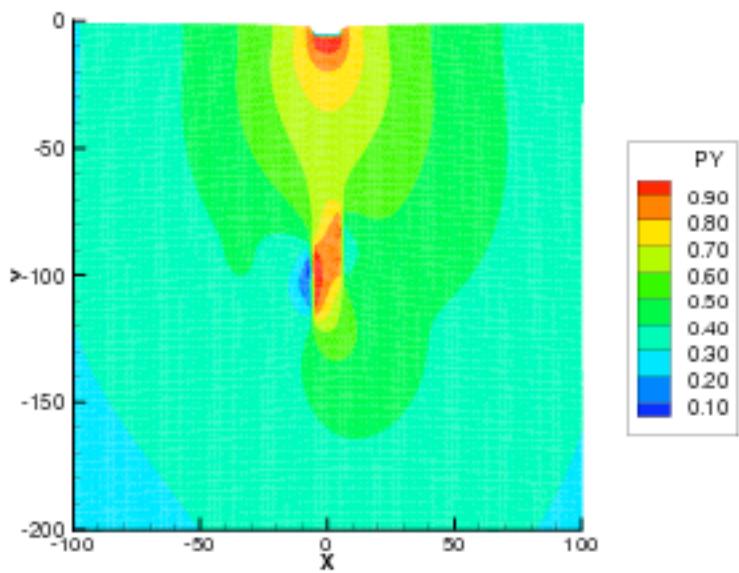


QC solution

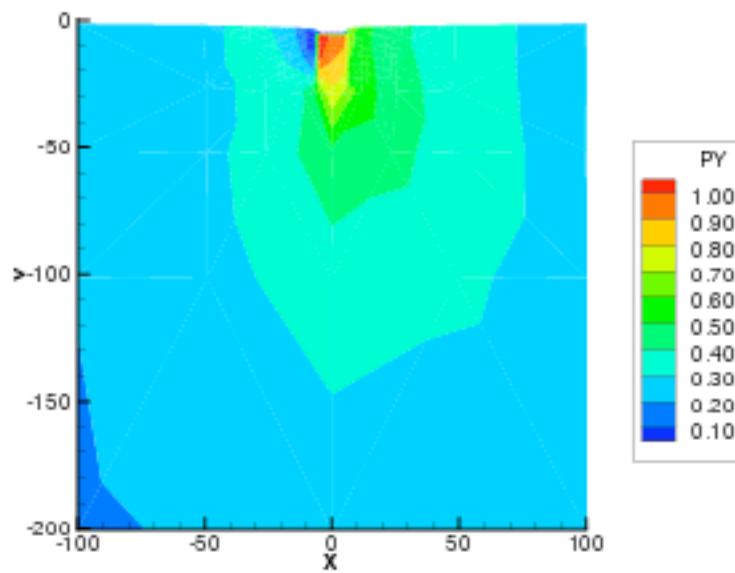
### 3. BASE AND QC DUAL SOLUTIONS

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Displacement in  $y$ -direction  
at dislocation nucleation



Base dual solution

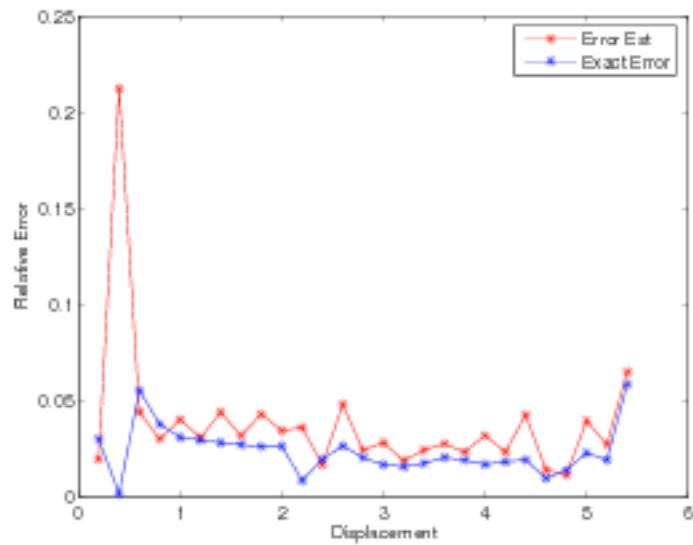
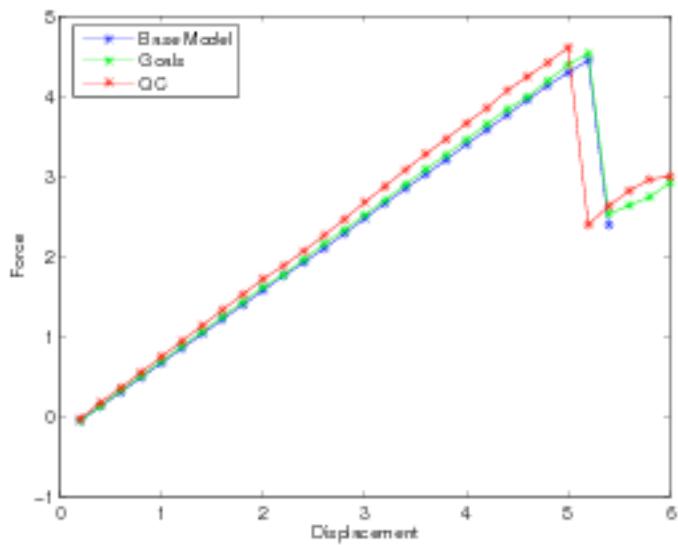


QC dual solution

**Observation:** An inaccurate  $u_0$  corrupts the dual solution.

### 3. FORCE-DISPLACEMENT AND ERROR CURVES

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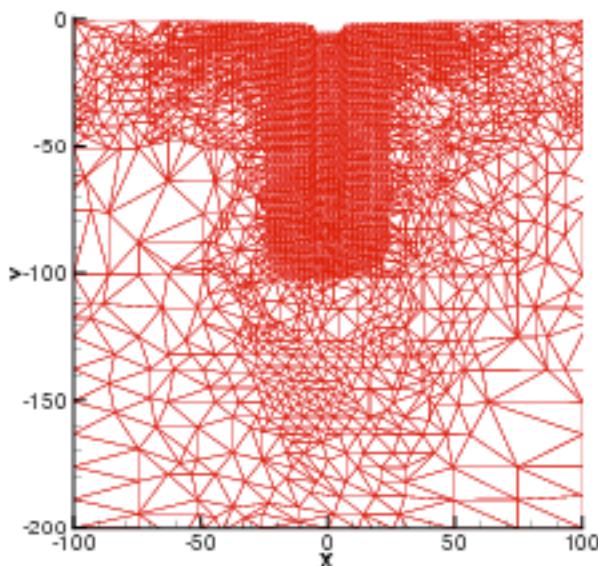
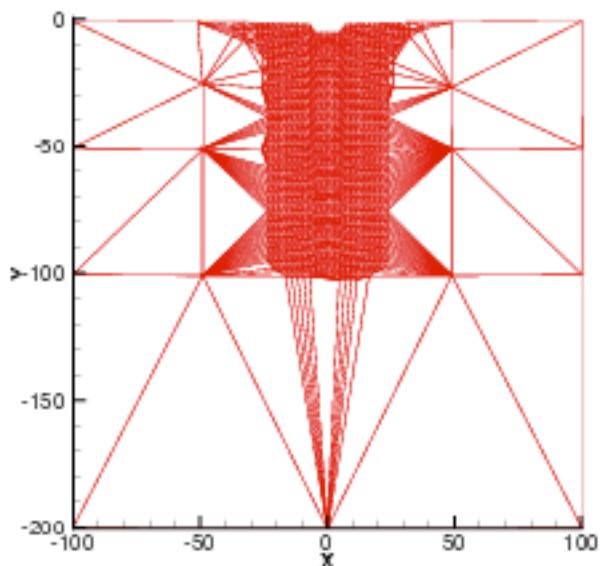


(Left) Force-displacement curve comparing the evolution of the base model, QC, and Goals solutions.

(Right) Exact and estimated relative errors for the Goals solution.

### 3. QC AND GOALS MESH ADAPTATION

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QC (left) and Goals (right) meshes at load step 27.  
(Right after the dislocation nucleation)

The numbers of atoms in the QC mesh and the Goals mesh are  
1629 and 3452.

### 3. MOLECULAR DYNAMICS EXAMPLE

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**The Base Model:** Let  $\Omega \subset \mathbb{R}^d$  and

$x_i$  = initial positions of  $n$  atoms in  $\bar{\Omega}$

$u_i$  = displacement of  $x_i$  at time  $> 0$

$M$  =  $n \times n$  mass matrix = diag  $\{m_i I_{(d \times d)}\}$

$V(u)$  = interatomic potential assumed to be given

$f(u) = -\partial_u V(u)$  = interatomic forces

**Find  $u$  such that**

$$M\ddot{u} = f(u), \quad \dot{u}(0) = V_0, \quad u(0) = U_0, \quad +B.C.$$

### 3. WEAK FORMULATION

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The solution  $u$  is assumed to belong to the space  $\mathbb{V}$ :

$$\mathbb{V} = C^2([0, T]; (\mathbb{R}^d)^n)$$

i.e.  $\forall t \in [0, T], v(t) \in V = (\mathbb{R}^d)^n$ .

**Weak formulation:**

**Find  $u \in \mathbb{V}$  such that  $B(u; v) = F(v), \quad \forall v \in \mathbb{V}$**

where:

$$\begin{aligned} B(u; v) &= \int_0^T v^T(M\ddot{u} - f(u))dt \\ &\quad + v^T(0)M\dot{u}(0) - \dot{v}^T(0)Mu(0) \end{aligned}$$

$$F(v) = v^T(0)MV_0 + \dot{v}^T(0)MU_0$$

### 3. THE DUAL PROBLEM

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**Find  $p \in \mathbb{V}$  such that  $B'(u; v, p) = Q'(u; v), \forall v \in \mathbb{V}$**

$$\begin{aligned} B'(u; v, p) = & \int_0^T (M\ddot{p} - (f'(u))^T p)^T v dt \\ & + (Mp)^T(T)\dot{v}(T) - (M\dot{p})^T(T)v(T) \end{aligned}$$

**Find  $p$  such that**

$$M\ddot{p} - (f'(u))^T p = 0, \quad -M\dot{p}(T) = q_f, \quad p(T) = 0$$

**with**

$$Q(u) = q_f^T u$$

**The entries of vector  $q_f$  are chosen such that  $Q(u)$  is an average of some component of  $u$  over several atoms at time  $T$ .**

### 3. THE SURROGATE MODEL

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**Bridging scale method\***: the goal is to develop a model s.t.:

1. MD is used only over a subdomain  $\Omega_{MD} \subset \Omega$
2. a coarse-scale model is used in  $\Omega_C = \Omega \setminus \Omega_{MD}$

**Averaging:** Let

1.  $V_h$  = space of piecewise linear functions
2.  $\pi$  = operator from  $V$  into  $V_h$
3.  $\mathcal{I}$  = “collocation” operator from  $V_h$  into  $V$



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\*Liu, Karpov, Zhang, and Park, CMAME 193 (2004)

\*Tang, Hou, and Liu, IJNME 65, 2006

### 3. THE SURROGATE MODEL

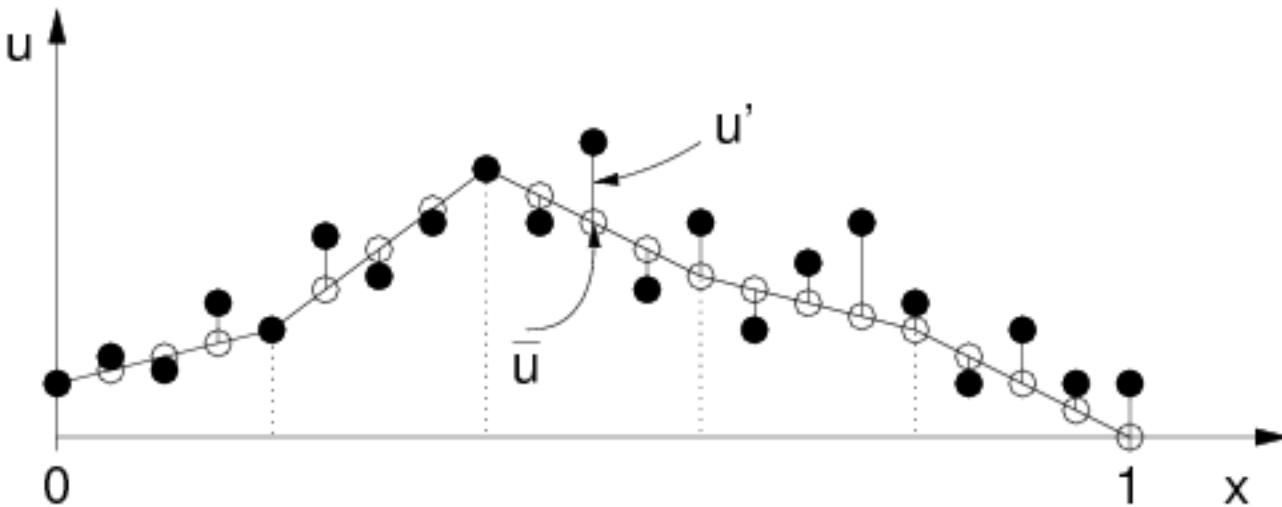
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The coarse scale displacements are constrained to be “piecewise linear”:

$$\bar{u} = \mathcal{I}\pi u = Pu$$

Decomposition of scales:

$$u = \bar{u} + u', \quad \bar{u} = Pu, \quad u' = (I - P)u = Qu$$



### 3. THE SURROGATE MODEL

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#### Issues

1. To choose the coarse-scale model to be consistent with the MD model.
2. To construct interface/boundary conditions for the MD models in  $\Omega_{MD}$ .

#### Coarse-scale dynamical model:

$$M_s \ddot{\delta} = \hat{f}(\delta), \quad \dot{\delta}(0) = v_0, \quad \delta(0) = u_0$$

where:

$$\delta = (\delta_1, \delta_2, \dots, \delta_s), \quad s \ll n.$$

$M_s$  =  $sd \times sd$ -mass matrix.

$\hat{f}$  =  $sd$ -vector of forces due to interatomic reactions.

### 3. ERROR ESTIMATE

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The solution of the surrogate model is given by:

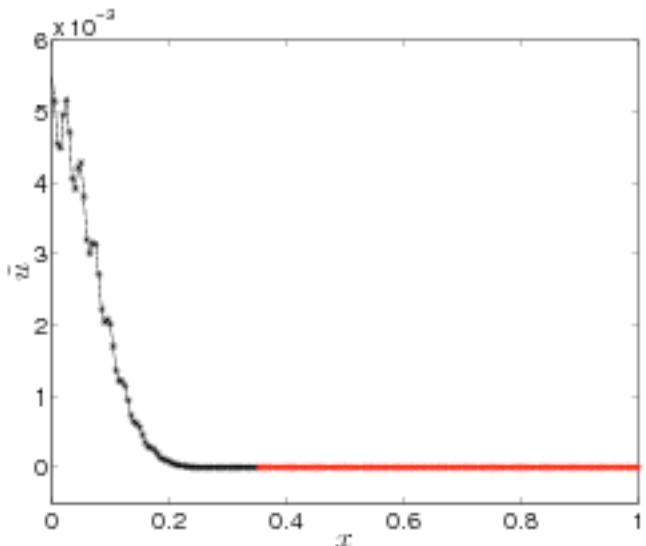
$$\tilde{u} = \begin{bmatrix} N\delta_C \\ N\delta_{MD} \end{bmatrix} + \begin{bmatrix} u'_G \\ u'_{MD} \end{bmatrix} \quad \begin{array}{ll} \text{in } \Omega_C \\ \text{in } \Omega_{MD} \end{array}$$

Define residual as:

$$\mathcal{R}(\tilde{u}, v) = \int_0^T v^T (\underbrace{M\ddot{\tilde{u}} - f(\tilde{u})}_{r(\tilde{u})}) dt = \int_0^T \sum_k v_k r_k(\tilde{u}) dt$$

$$\begin{aligned} Q(u) - Q(\tilde{u}) &\approx \mathcal{R}(\tilde{u}, p) = \int_0^T \left[ \sum_k p_k r_k(\tilde{u}) \right] dt = \int_0^T \eta_t dt \\ &= \sum_k \left[ \int_0^T p_k r_k(\tilde{u}) dt \right] = \sum_k \eta_k \end{aligned}$$

### 3. NUMERICAL EXAMPLE\*



Initial Displacement  $u_0$

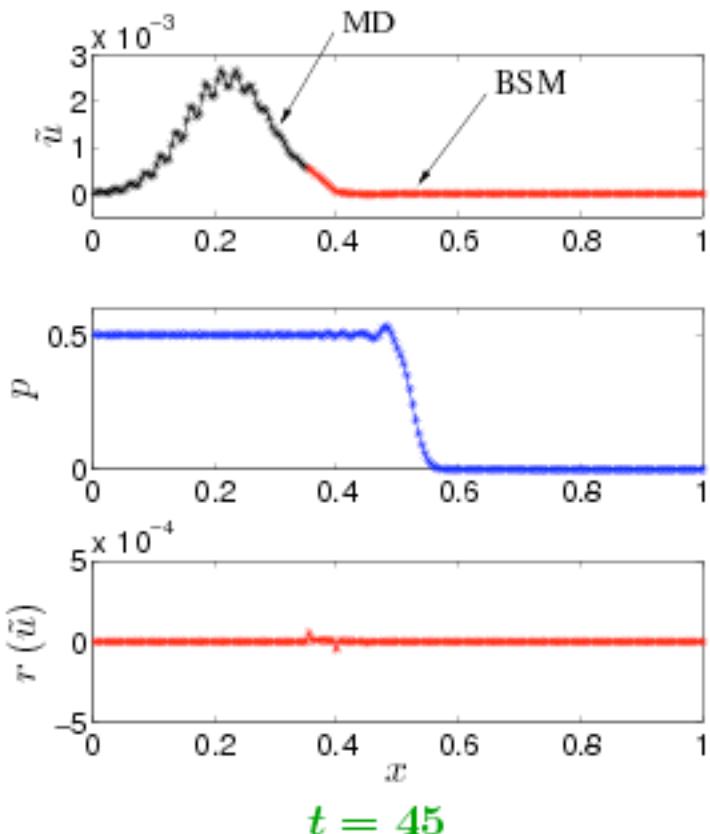
- ▶  $\Omega = [-2, 2], \Omega_{MD} = [-.35, .35]$
- ▶  $u(0) = u_0, u = 0$  on  $\partial\Omega$
- ▶  $f(u) = Ku$ , linear springs
- ▶  $Q(u) = \frac{1}{|\mathcal{M}|} \sum_{i \in \mathcal{M}} u_i$  where  
 $\mathcal{M} = \{i : |x_i| \leq .0025\}$

\*G. Wagner and W. K. Liu, J. Comp. Phys. 190, (2003)

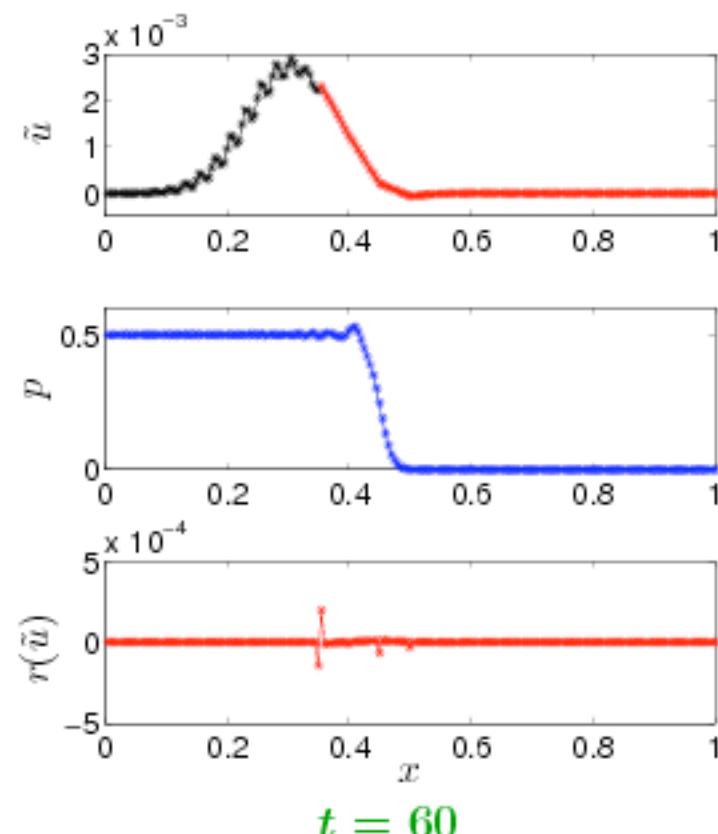
\*S. Tang, T. Y. Hou, W. K. Liu., IJNME 65, 2006

### 3. SOLUTIONS

#### Time Snapshots of Primal, Dual, and Force Residual\*



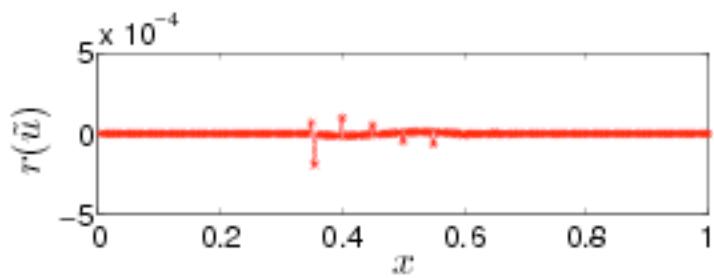
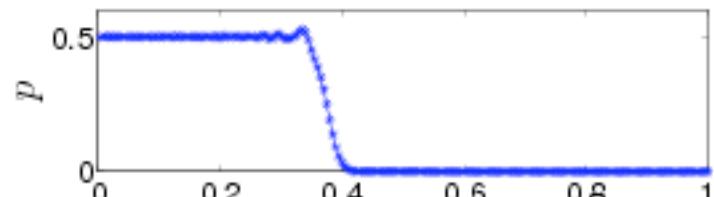
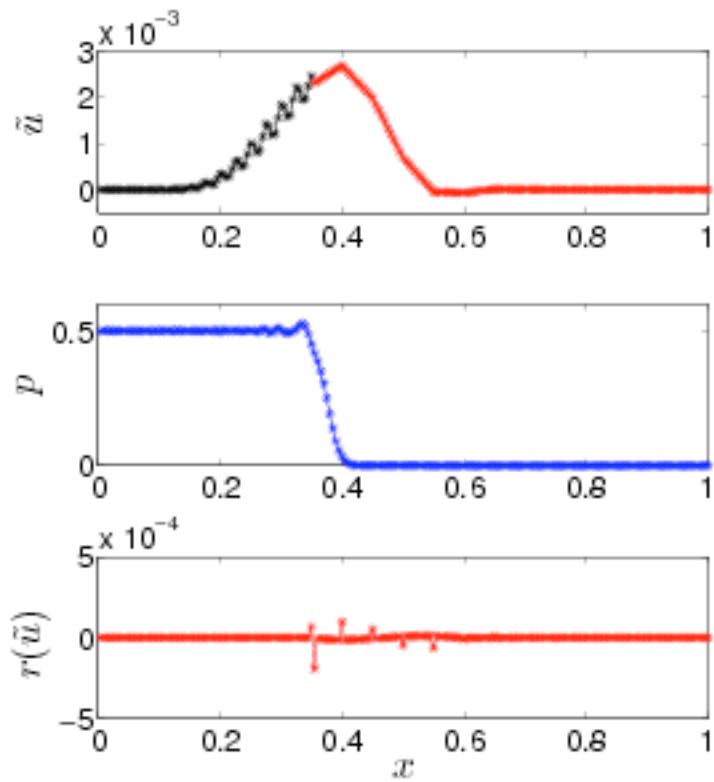
\* Note that  $\mathcal{E} = Q(u) - Q(\tilde{u}) = p * r(\tilde{u})$



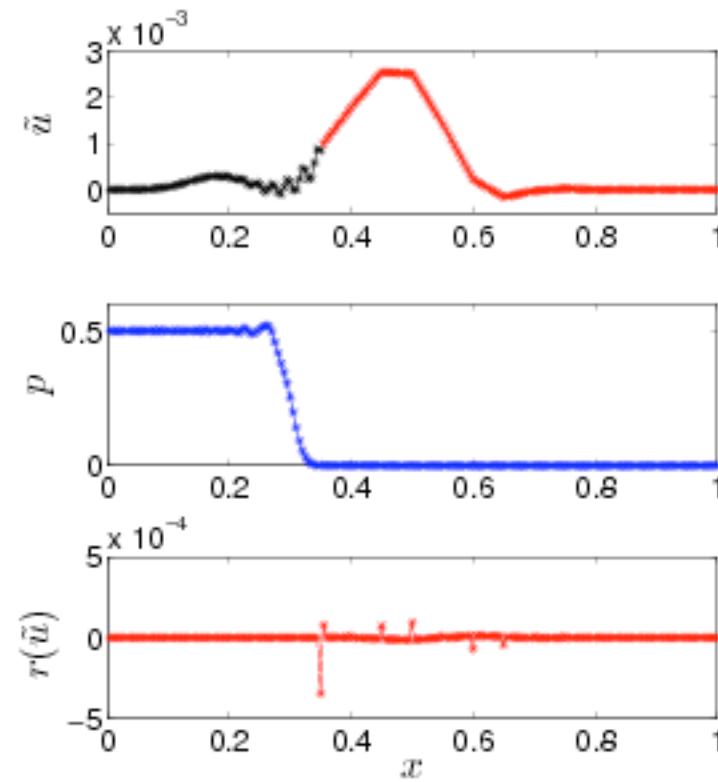
### 3. SOLUTIONS

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#### Time Snapshots of Primal, Dual, and Force Residual



$t = 75$

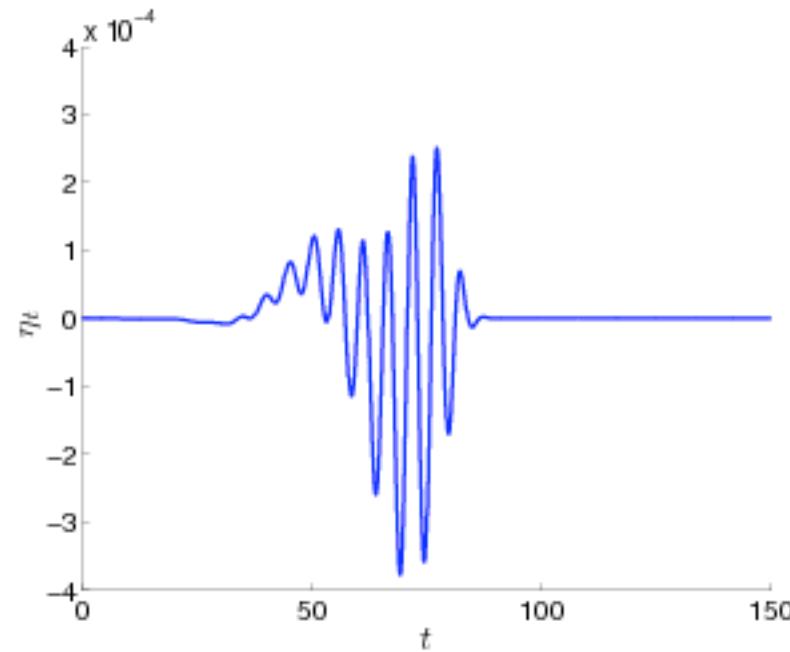


$t = 90$

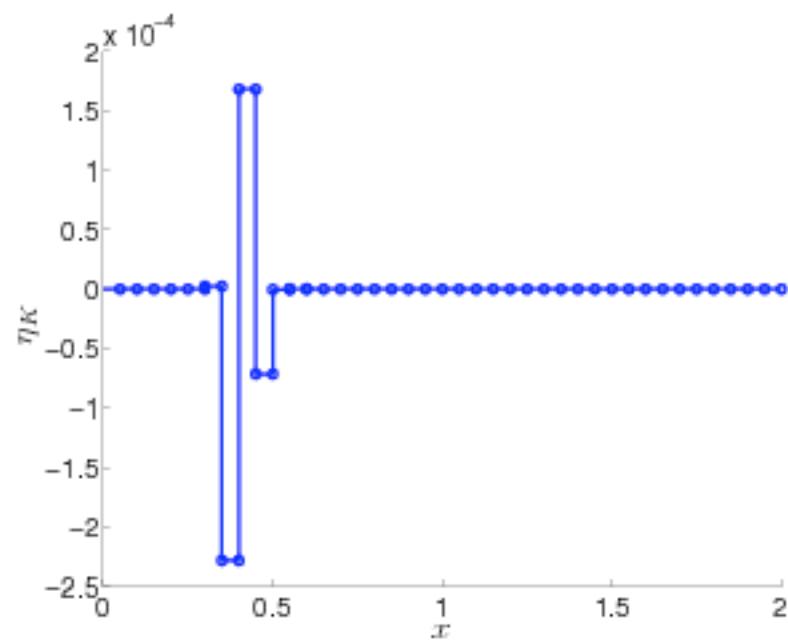
### 3. ERROR ESTIMATE

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Temporal Contribution to  
the error in the QoI



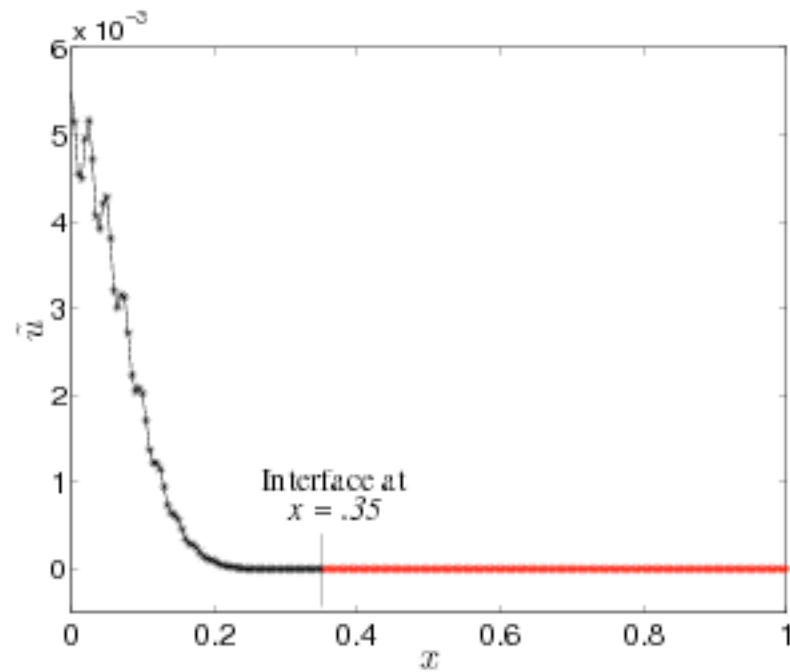
Spatial Contribution to  
the error in the QoI



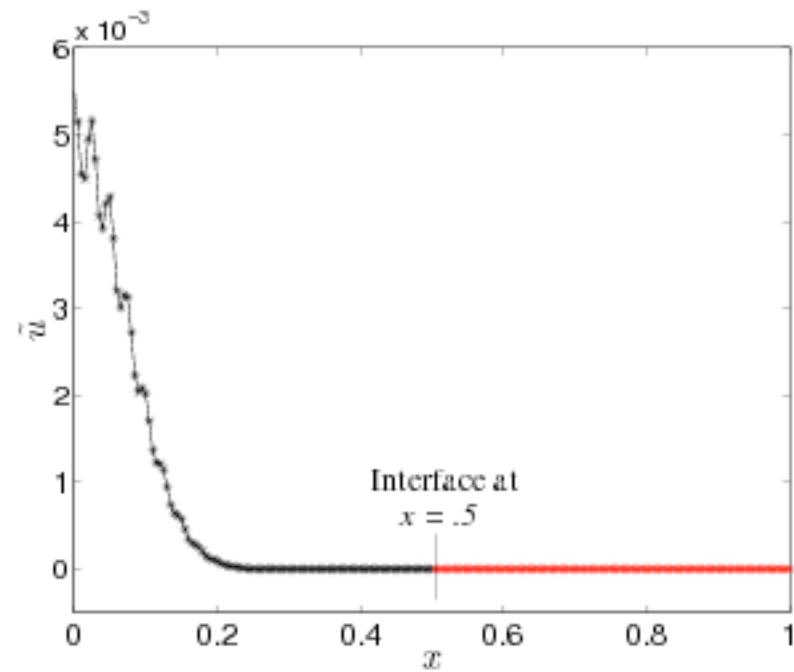
### 3. ADAPTATION: ONE STEP OF GOALS ALGORITHM

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Before Adaptation

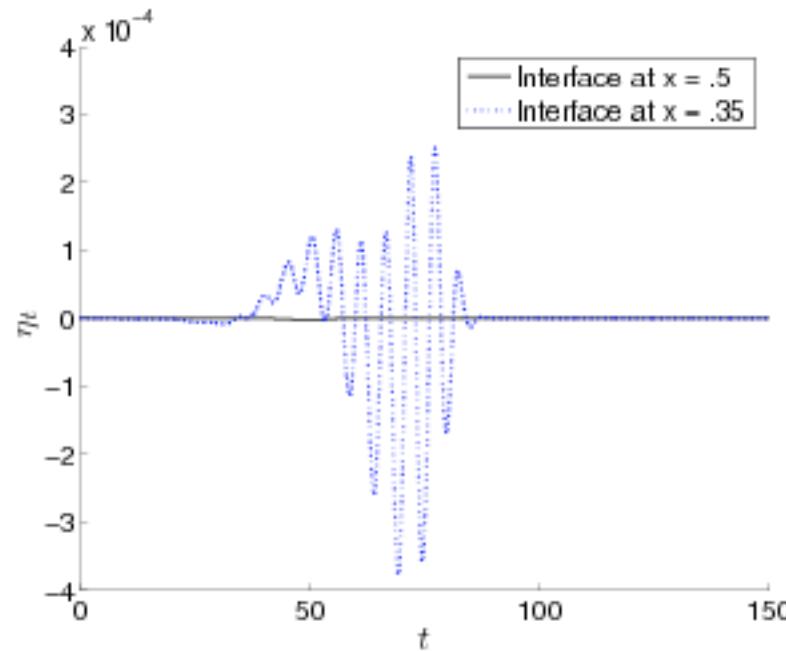


After Adaptation

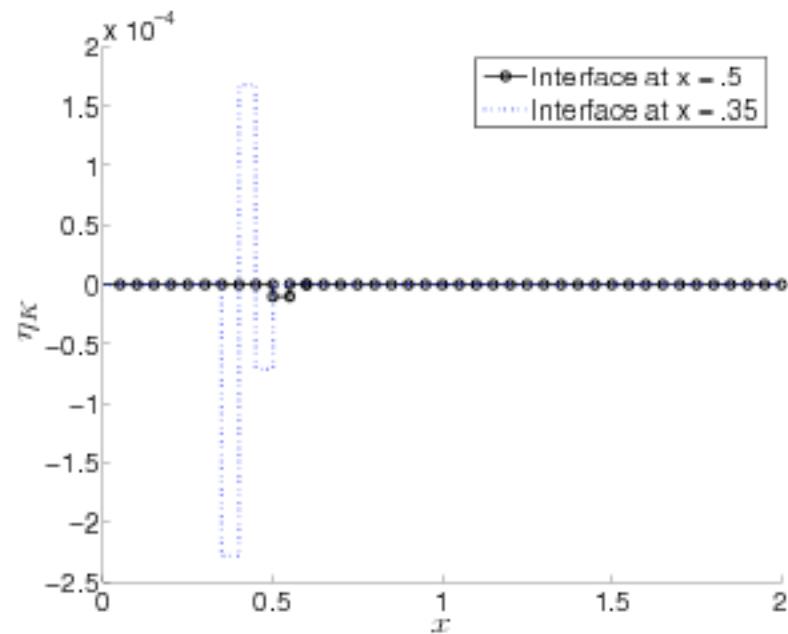


### 3. ADAPTATION: ONE STEP OF GOALS ALGORITHM

Temporal Contribution to  
the error in the QoI

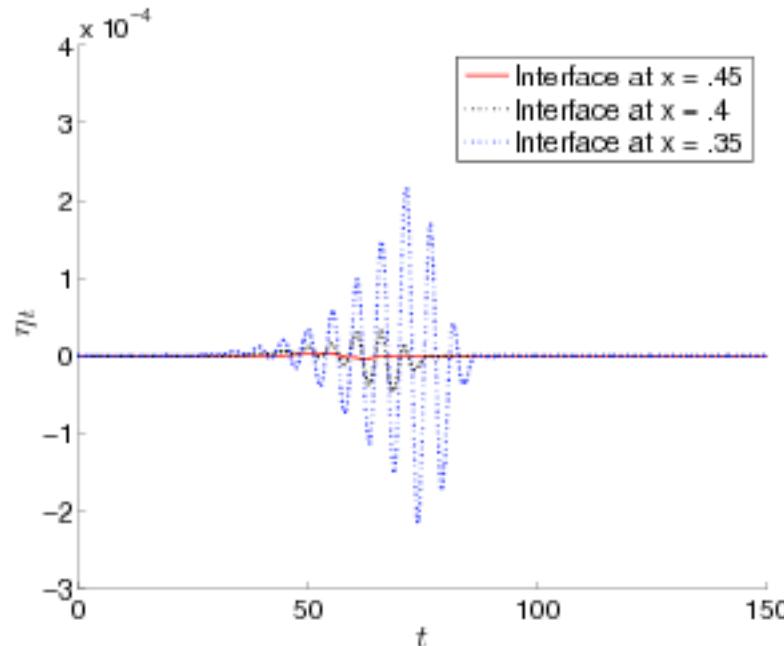


Spatial Contribution to  
the error in the QoI

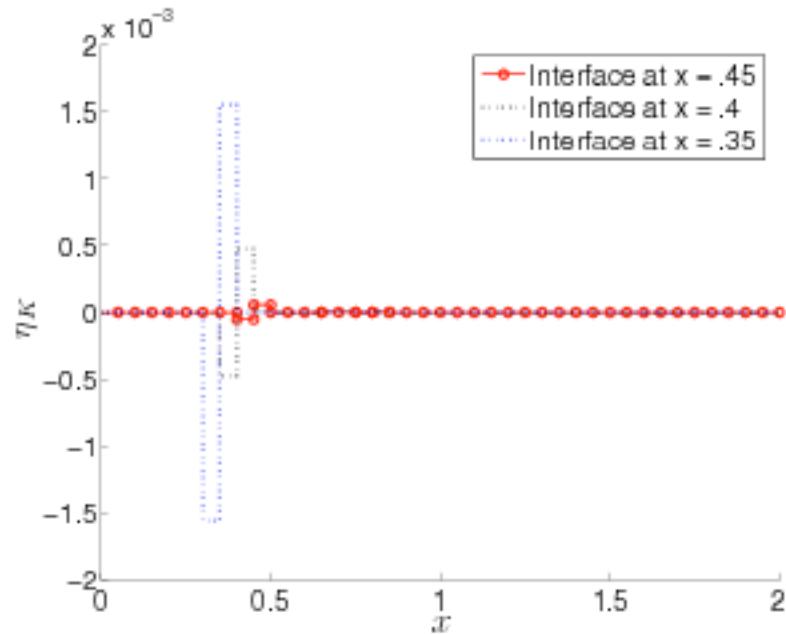


### 3. PMM\*: TWO STEPS OF GOALS ALGORITHM

Temporal Contribution to  
the error in the QoI



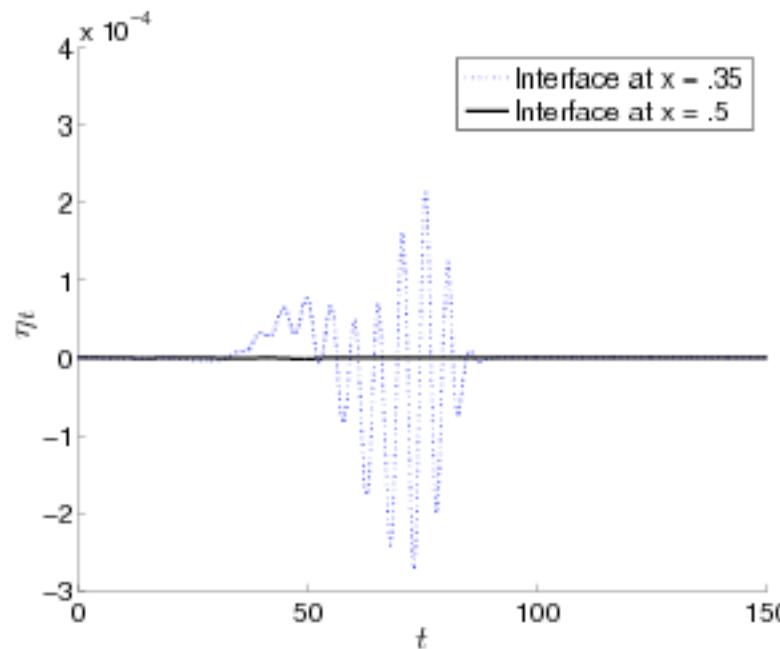
Spatial Contribution to  
the error in the QoI



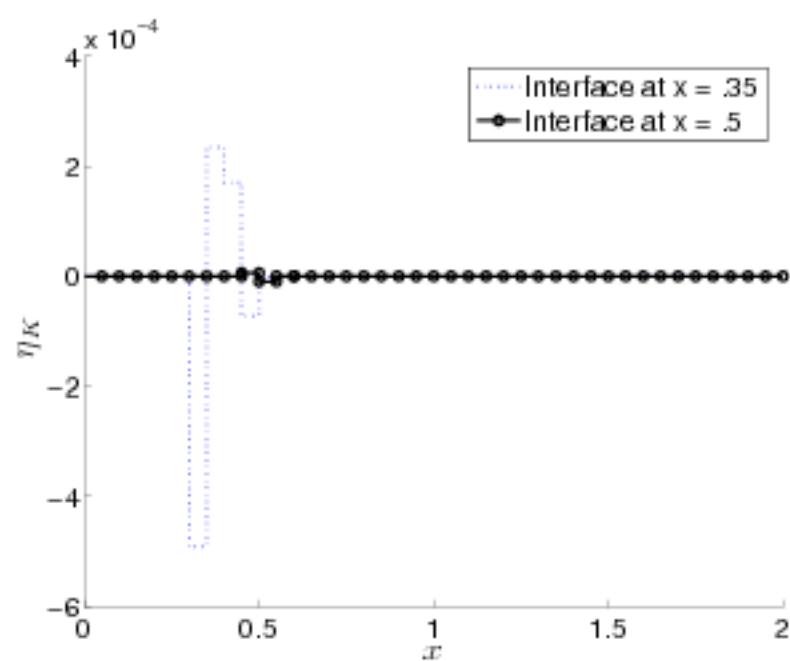
\**Pseudo-spectral Multi-scale Method – S. Tang, T. Y. Hou, & W. K. Liu,  
JCP 213, 2006*

### 3. BSM – NONLINEAR POTENTIAL\*

Temporal Contribution to  
the error in the QoI



Spatial Contribution to  
the error in the QoI

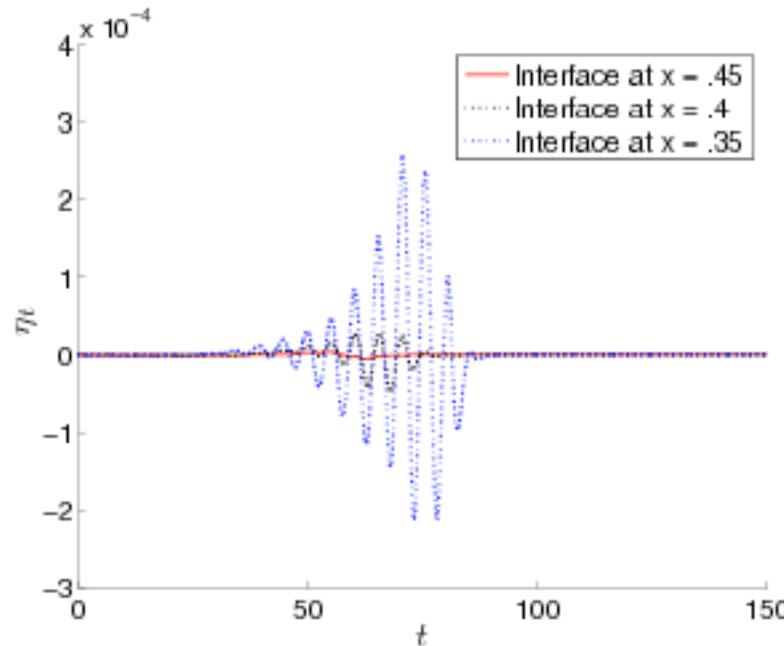


$$* U(u) = \frac{1}{2} \sum_n (u_{n+1} - u_n)^2 + \frac{K}{4} [(u_{n+1} - u_n)^4], K \in \mathbb{R}$$

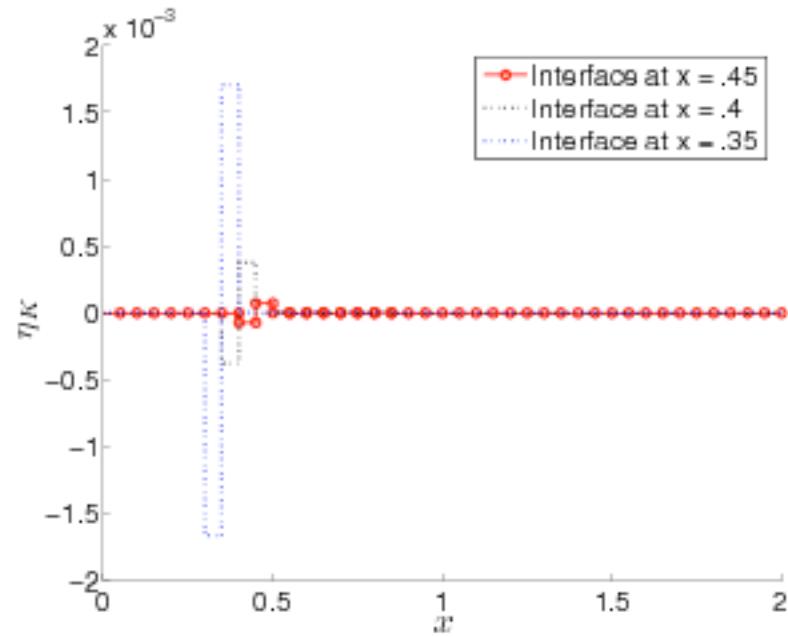
see Tang, Hou & Liu, IJNME 65, 2006.

### 3. PMM – NONLINEAR POTENTIAL\*

#### Temporal Contribution to the error in the QoI



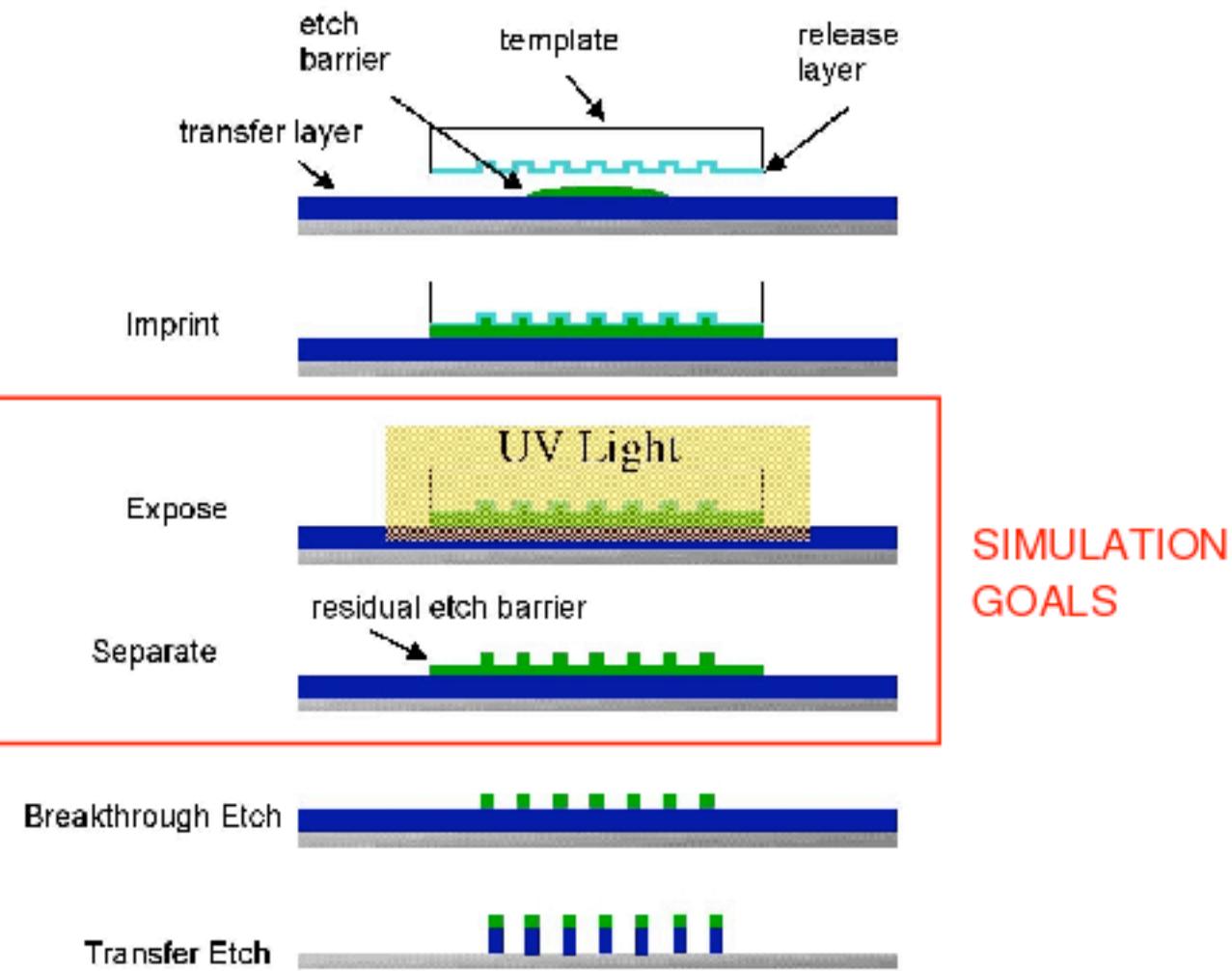
#### Spatial Contribution to the error in the QoI



\*  $U(u) = \frac{1}{2} \sum_n (u_{n+1} - u_n)^2 + \frac{K}{4} [(u_{n+1} - u_n)^4]$ ,  $K \in \mathbb{R}$

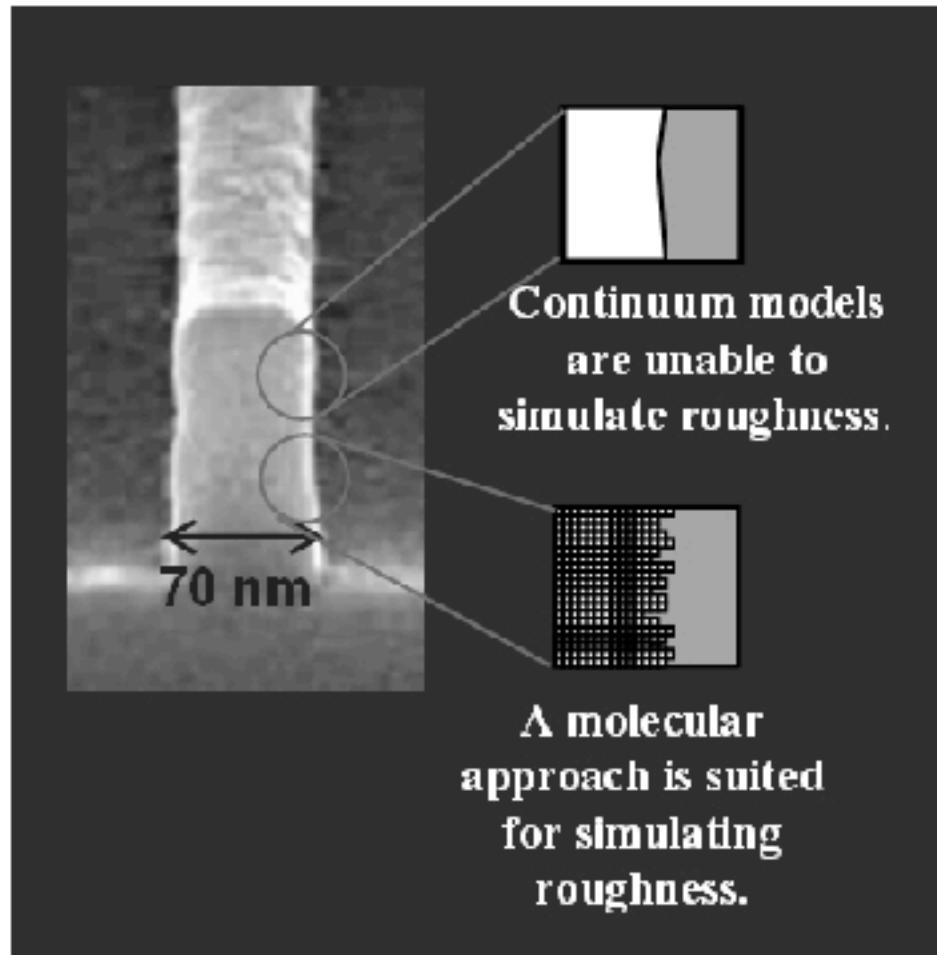
see Tang, Hou & Liu, JCP 213, 2006.

## 4. STEP AND FLASH IMPRINT LITHOGRAPHY



## 4. CONTINUUM/MOLECULAR MODELING

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## **4. EXPOSURE AND SEPARATION**

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The process is modeled in two steps:

**1. Polymerization step:**

The etch barrier is a mixture composed of initiators, monomers, crosslinkers. Upon UV exposure, the mixture undergoes free radical polymerization. This stage is modeled by a Monte-Carlo algorithm to determine the covalent bonds.

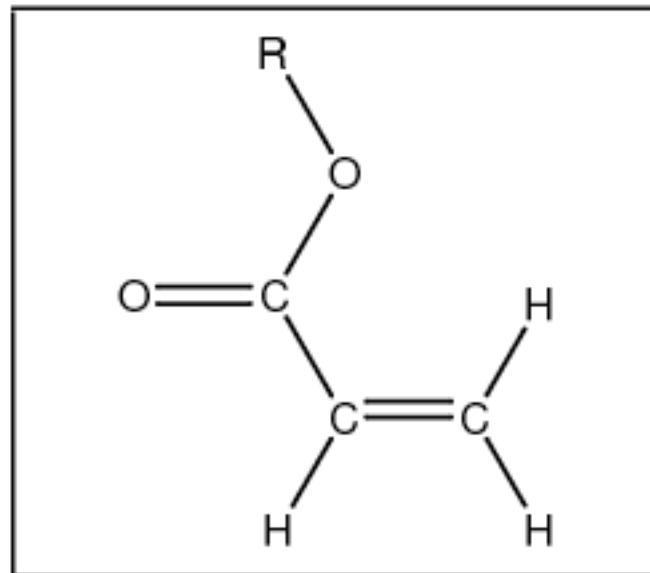
**2. Densification step:**

The etch barrier, upon polymerization, undergoes a bulk deformation resulting in a reduction of volume. This stage is modeled by a molecular statics approach in which bonds are represented by harmonic and Lennard-Jones springs.

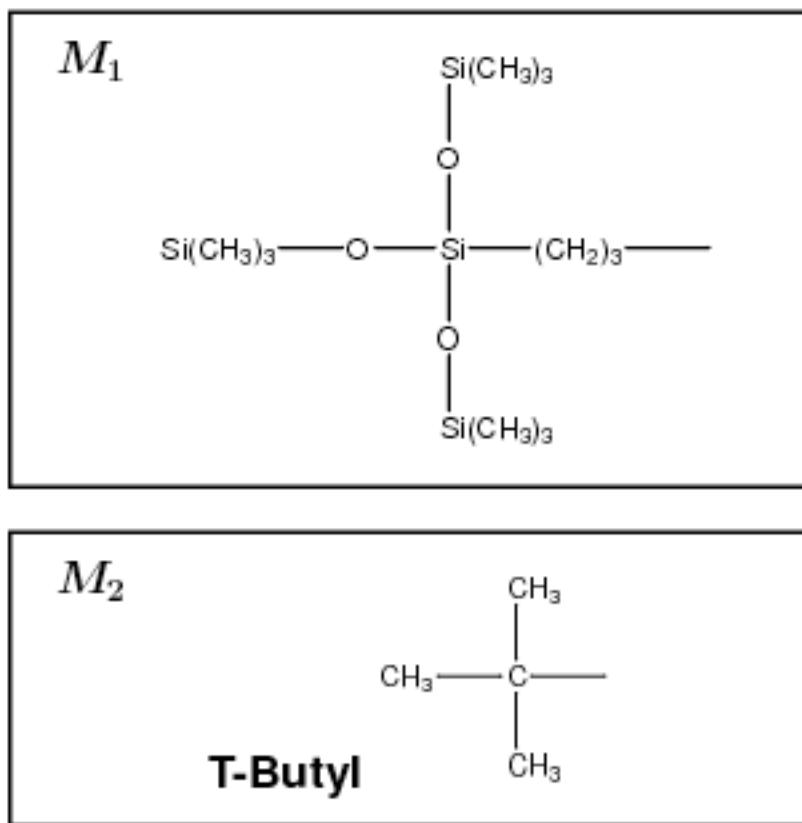
## 4. POLYMER

The polymer is made from a mixture of two acrylate-based monomers:

1.  $M_1$  = silicon monoacrylate (Gelest SIA-0210) for etch resistance
2.  $M_2$  = t-Butyl acrylate (TBA) to maintain low viscosity



**Acrylate**

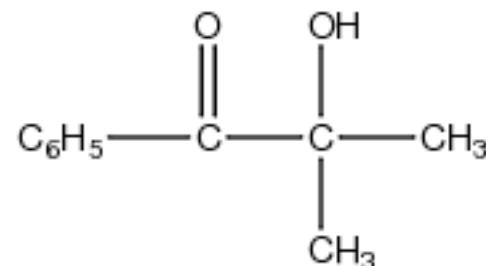


## 4. POLYMER

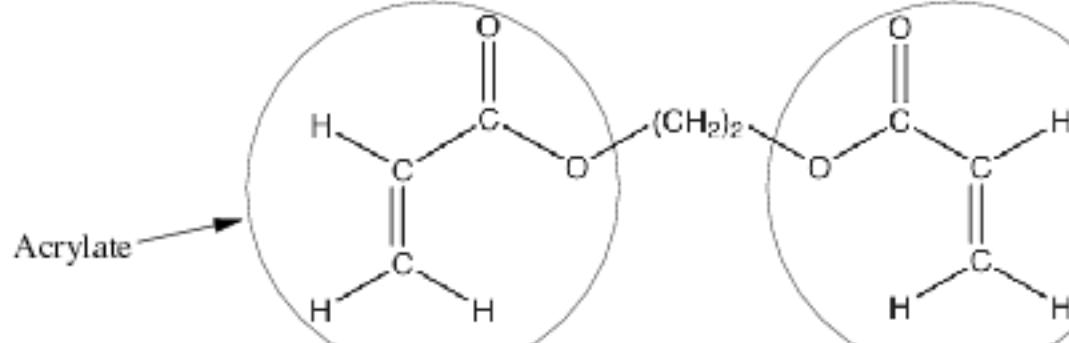
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The mixture also contains:

1. A photo-initiator  $I$ :



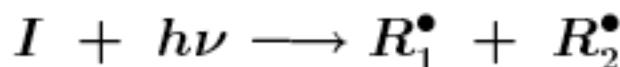
2. A cross-linker  $X_L$ :



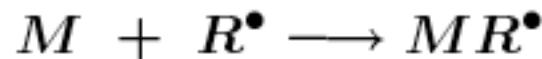
## 4. REACTIONS AND RATES

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### Initiation:



### Propagation:



### Termination:



### Rates:

$$\frac{d[I]}{dt} = -k_I \varphi_m [I]$$

$$\frac{d[R]}{dt} = -2k_I \varphi [I] - 2k_t [R]^2$$

$$\frac{d[M]}{dt} = -k_p [M][R]$$

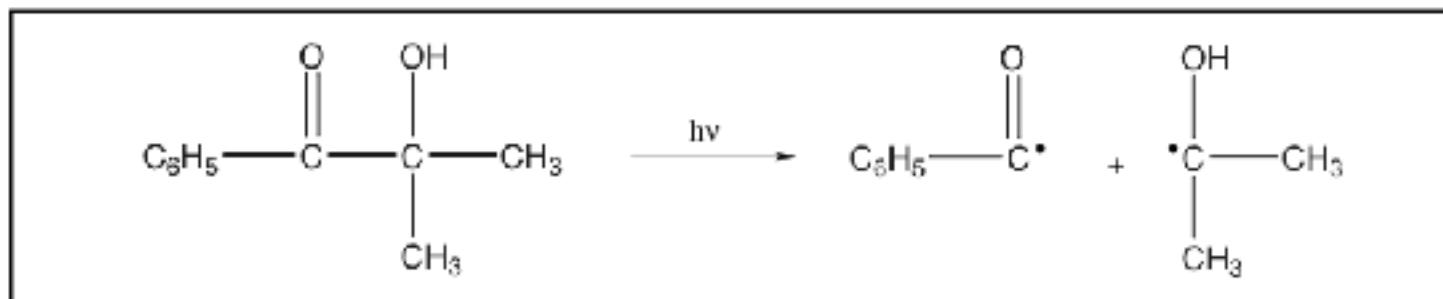
### Arrhenius Law:

### **Canonical Ensemble**

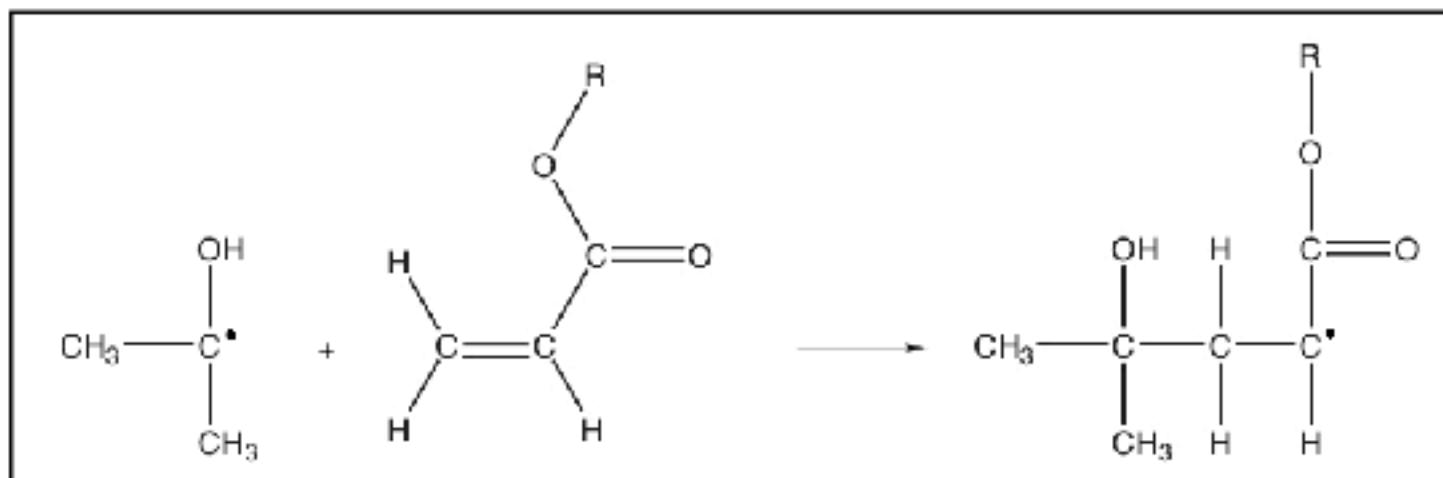
$$P = Ce^{-E_a/\kappa T} \propto k$$

## 4. EXAMPLES OF REACTIONS

**Initiation:**



**Propagation:**



## 4. KINETIC MONTE-CARLO ALGORITHM

### 1. Lattice cell placement:

- a) Boundary cells.
- b) Each lattice site assigned a constituent according to a random number,  $0 \leq r \leq 1$ .
- c) Random swapping process.

### 2. Initialization loop:

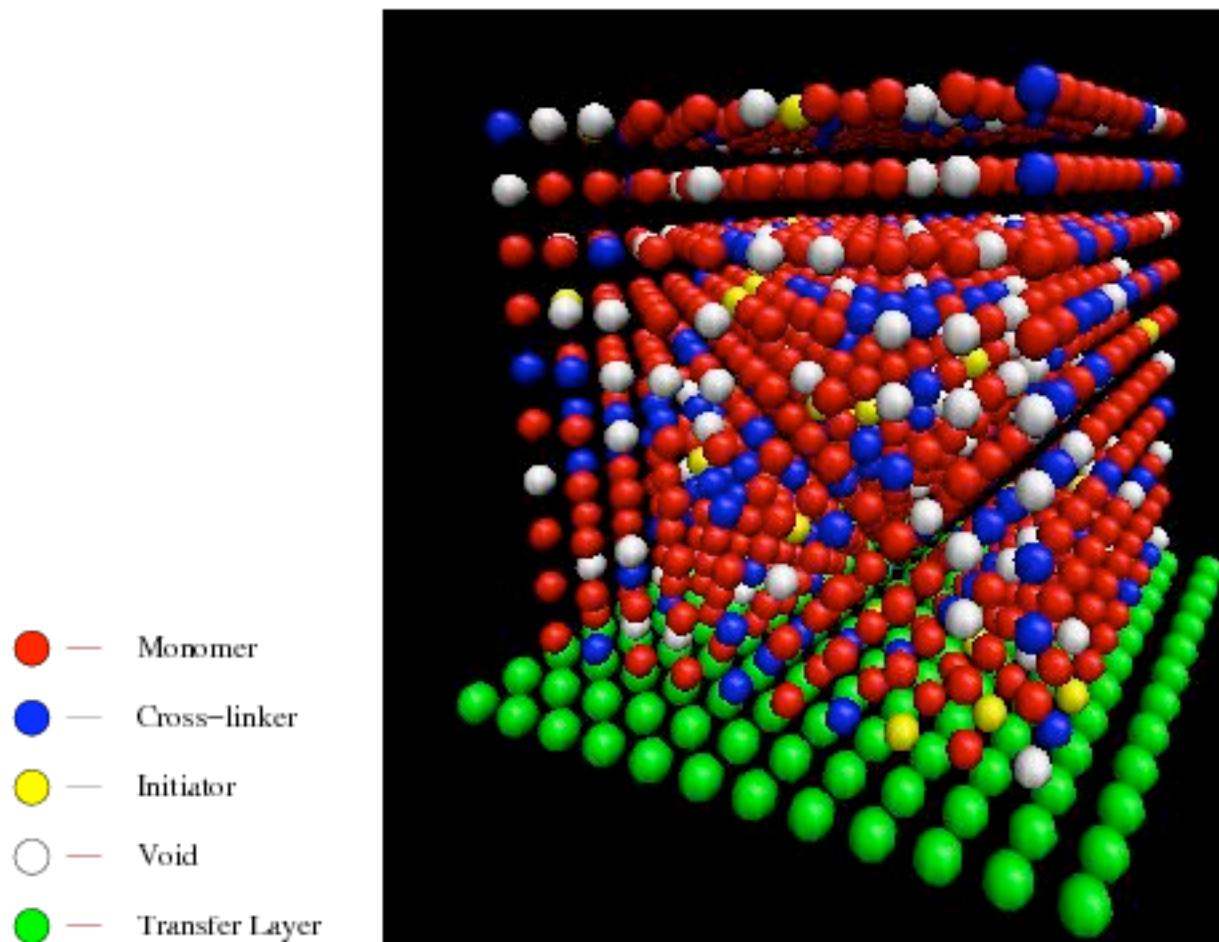
- a) Select a random lattice site and check if initiator.
- b) If yes, initiator reacts into a radical if  $r < P_I$ .
- c) Repeat  $N_I$  times.

### 3. Propagation loop:

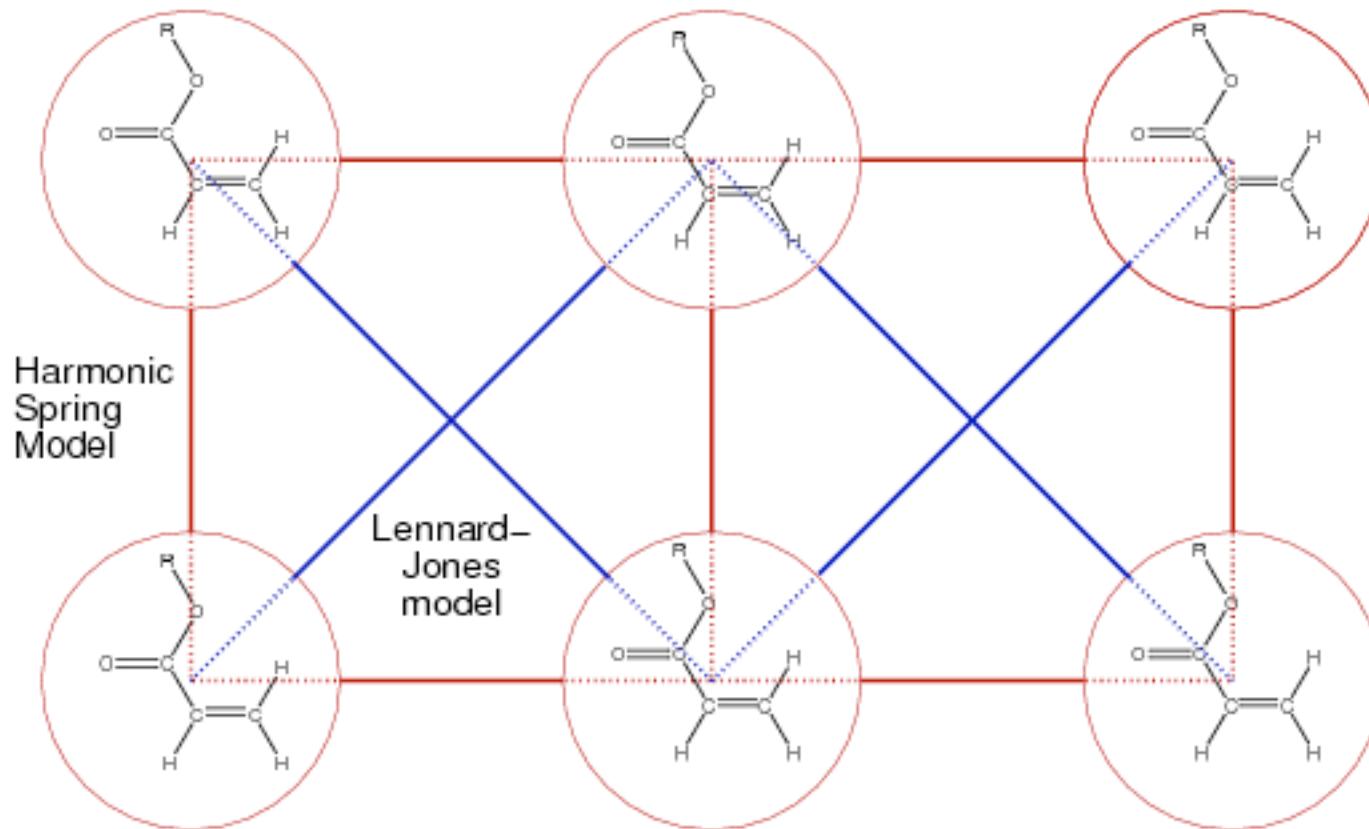
- a) Select a random site in lattice.
- b) If void, do nothing.
- c) If initiator, make it react if  $r < P_I$ .
- d) If radical, select a random neighbor. Radical reacts with neighbor  $n$  if  $r < P_n$ . If  $n$  is not connected to a radical, this is a propagation step, otherwise, a termination step.
- e) If unbonded particle (different from void, initiator, active radical) and neighbor is void, switch void and particle.
- f) Repeat  $N_p$  times.

## 4. POLYMER NETWORK

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## 4. MATHEMATICAL MODEL



**ISSUE: DETERMINE SPRING CONSTANTS**

## 4. MATHEMATICAL MODEL: MOLECULAR STATICS

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**Given:**

Lattice with  $N$  particles, whose position is  $\mathbf{x}_i$  each particle has  $N_i$  neighbors, the energy between particle  $i$  and a neighbor  $j$  is  $E_{ij}(\mathbf{x}_i, \mathbf{x}_j)$

**Goal:**

**Find**  $\mathbf{x}^* = \min_{\mathbf{x}} E(\mathbf{x})$ , where  $E(\mathbf{x}) = \sum_{i=1}^N \sum_{j=1}^{N_i} E_{ij}(\mathbf{x}_i, \mathbf{x}_j)$

$$\Rightarrow \frac{\partial E(\mathbf{x}^*)}{\partial \mathbf{x}} = \mathbf{F}(\mathbf{x}^*) = 0$$

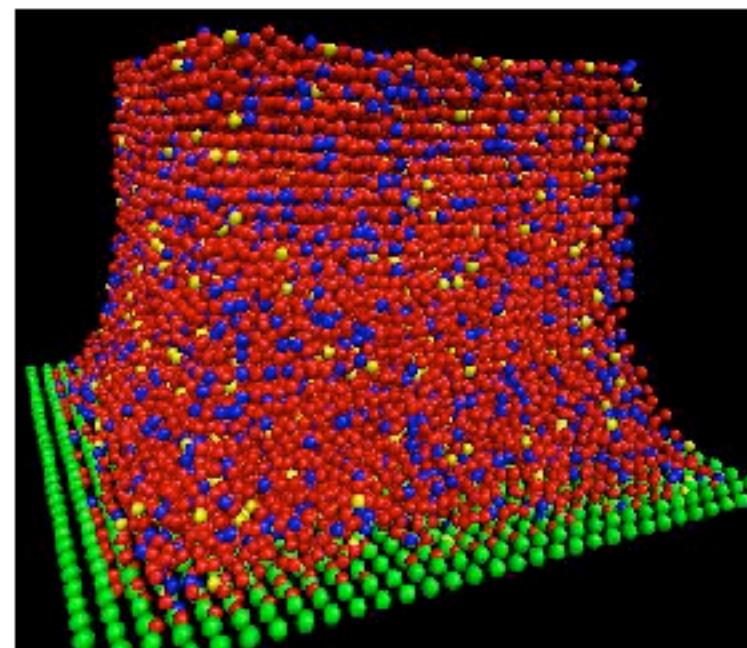
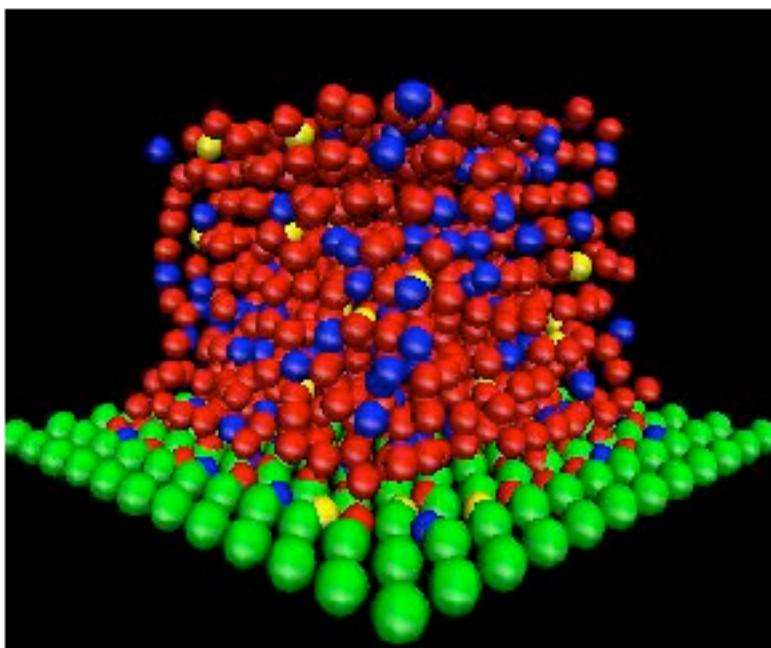
## 4. ALGORITHM: INEXACT NEWTON-CG WITH LINE SEARCH

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1. Initialize lattice
2. set  $s=0$
3. Compute  $F(x_s)$ , and  $\frac{\partial F}{\partial x_s}(x_s)$
4. Solve  $\frac{\partial F}{\partial x_s} \Delta x = -F$  using PCG. Terminate PCG when:
  - ▶ PCG tolerance reached
  - ▶ Negative curvature detected
5. Perform line search for  $\alpha$ :  $\min_{\alpha} E(x_s + \alpha \Delta x)$
6.  $x_{s+1} = x_s + \alpha \Delta x$
7.  $s = s+1$
8. Stop when  $\|F(x_s)\| < \epsilon$

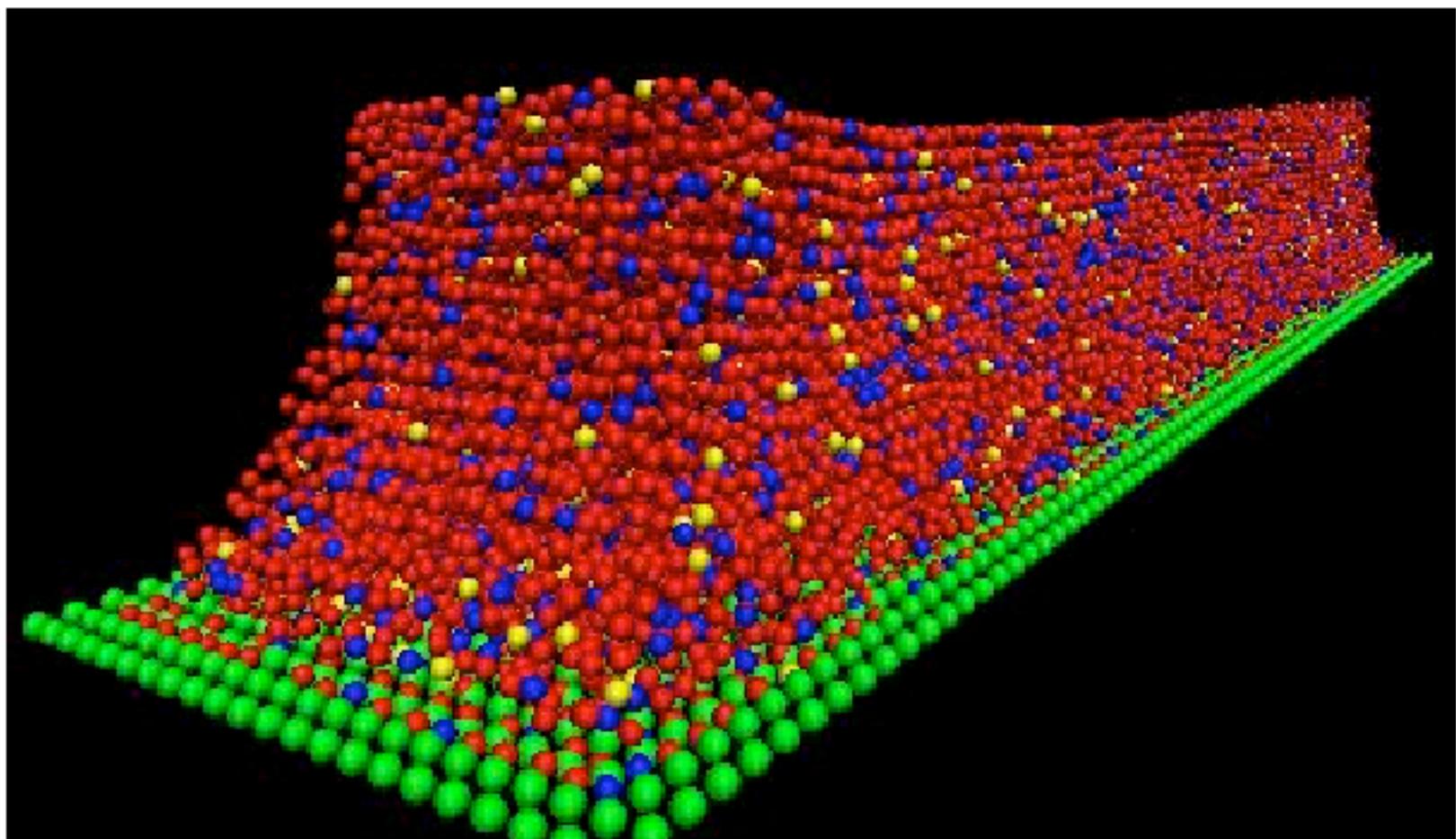
## 4. PRELIMINARY RESULTS

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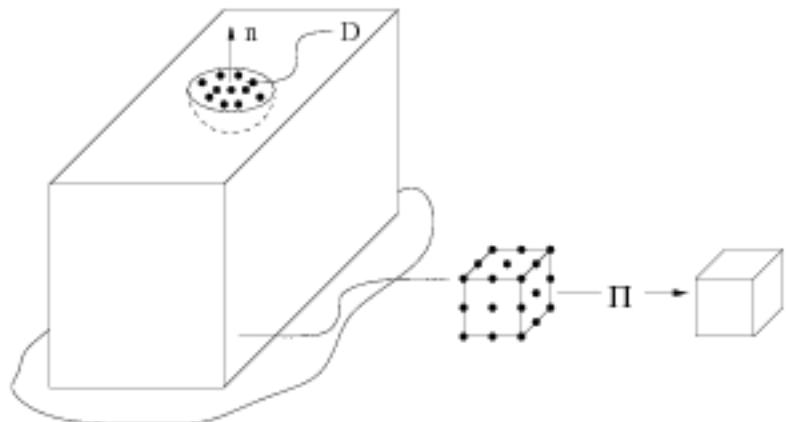
## 4. PRELIMINARY RESULTS

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## 4. POSSIBLE MULTI-SCALE APPROACHES FOR SFIL

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$$Q(\mathbf{u}) = \frac{1}{|D|} \sum_{j \in I_D} \mathbf{u}_j \cdot \mathbf{n}$$

### 1. Hierarchical

$$W = \sum_r \sum_s \sum_t C_{rst} (I_C - 3)^r (II_C - 3)^s (III_C - 3)^t$$

### 2. Concurrent

Use above model concurrently with molecular model

### 3. *hp*-quasicontinuum

## 5. CONCLUSIONS

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- ▶ Estimation of error in **quantities of interest** can be used as a basis for **model adaptivity** via Goals-type algorithms.
- ▶ In atomistic-continuum models, the properties of the continuum must reflect appropriately those of the microstructure or **modeling error** can be large and difficult to control.
- ▶ The construction of the **base** atomistic/molecular model can be a computational problem of complexity equal to solving the model itself.
- ▶ The construction of viable surrogate models still involves the resolution of the **interface** problem.
- ▶ Many **fundamental** mathematical and computational problems remain open.